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EXHIBIT B

Vashishta et al. "Giant Molecular Dynamics Simulations of Nanopixels" as available at

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More Science Successes

Giant Molecular Dynamics Simulations of Nanopixels

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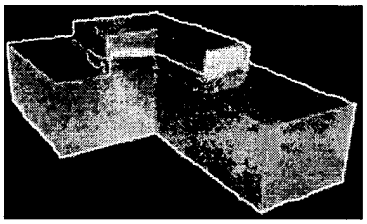
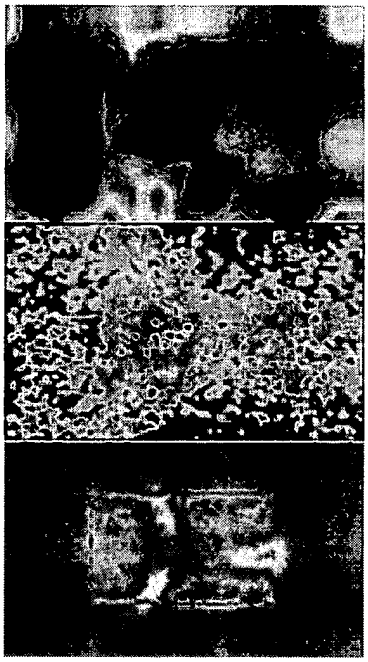
Silicon nitride deposited on silicon is used as a dielectric layer in semiconductor technology because of its high density, high dielectric constant, and resistance to radiation damage. The process for producing a silicon nitride layer is plasma-enhanced chemical vapor deposition followed by annealing. This produces an interface that is usually amorphous, but occasionally crystalline. When it is crystalline, the lattice structures of the silicon and the silicon nitride match nearly perfectly.





Stress in a Nanopixel

Above: Stress distribution in a nanopixel on a silicon substrate. One quarter is removed to show internal stresses. Right: Horizontal cross-sections of stress in nanopixels covered with amorphous silicon nitride through Si3N4 above the interface (top), Si mesa below the interface (middle) and substrate (bottom). Tensile stress maximum is -2 GPa (blue), compressive stress maximum is +2 GPa (red).

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Giant Molecular Dynamics Simulations of Nanopixels

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But not perfectly enough. Lattice-mismatch-induced stresses can cause defects and adversely affect the electronic properties of nanodevices--and the smaller these tiny layered devices become, the less predictable the effects. The continuum finite-element calculations typically used to study stress effects cannot fully resolve them over the tiny volumes involved, so scientists have turned to atomistic molecular dynamics simulations.

A group at Louisiana State University in Baton Rouge has recently carried out the first multimillion-atom molecular dynamics simulations of stresses in silicon/silicon nitride "nanopixels," representations of devices only 50 nanometers square by 10 nanometers high. The simulations were carried out on the HP Exemplar at Caltech, distributed over 128 of the 256 processors. Their results were reported in Applied Physics Letters.

The Louisiana State University team consists of Martina E. Bachlechner, Ingvar Ebbsjö (Uppsala University), Rajiv K. Kalia, Aiichiro Nakano, Andrey Omeltchenko, and Priya Vashishta. In this project, they collaborated with Anupam Madhukar of the University of Southern California and Paul Messina of Caltech.

In their simulations, the stress concentration is observed near the interface and at the mesa/substrate edges. A lattice mismatch of 1.1% at the Si(111)/Si3N4(0001) interface manifests as a stress well at the center of the mesa.

In contrast to the crystalline case, the stresses in the case of amorphous Si3N4 are highly inhomogeneous along the interface. Below the interface, tensile stress domains separated by compressive domain walls are observed in silicon. The spatial extent of these stress domains is and maximum tensile and compressive stresses in the domains and domain walls are -2 GPa and +2 GPa, respectively.

The computations involved 10 million atoms, used 100 MB per node of memory, and took from 30 to 60 hours of wall clock time per simulation–a total of four different simulations were carried out.

REFERENCES

M.E. Bachlechner, A. Omeltchenko, A. Nakano, R.K. Kalia, P. Vashishta, A. Madhukar, and P. Messina: Multimillion-atom molecular dynamics simulation of atomic level stresses in Si(111)/Si3N4(0001) nanopixels, Applied Physics Letters 72, pp. 1969-1971 (20 April 1998).